Stats 318: Lecture # 11

Agenda: MCMC

- Cluster algorithms
- The Swendsen-Wang algorithm
- The Wolff’s algorithm
- Application to the Ising model
Gibbs sampling

- Wish to sample from $\pi(x_1, \ldots, x_n)$
- Partition coordinates into subgroups $g_1, \ldots, g_k$: $\pi(x_{g_1}, \ldots, x_{g_k})$
- Pick a subset and resample group of coordinates $X_g$ given other coordinates

  e.g. 2 blocks

  Repeat

- Sample from $\pi(x_{g_1} \mid x_{g_2})$
- $\pi(x_{g_2} \mid x_{g_1})$

  Until convergence
Phase transition in Ising model

\[ \pi(x) \propto \exp \left( \beta \sum_{v \sim v'} x_v x_{v'} \right) \]
\[ \beta = \frac{1}{T} \]

- When temperature is high, all spins behave nearly independently (no long-range correlation)
- When temperature is below a critical temp \( T_c \), all the spins tend to be aligned (cooperative performance)
- Single site update Gibbs sampler slows down rapidly once \( T \) is approaching \( T_c \) or is below \( T_c \): e.g.
  \[ \mathbb{P}(X_v = -1 \mid \text{neighbors} = +1) = (1 + e^{2\beta \# \text{neighbors}})^{-1} \ll 1 \]
- Swendsen & Wang algorithm almost completely eliminates critical slow down
Data augmentation

$$\pi(x) \propto e^{\beta \sum_{v \sim v'} x_v x_{v'}} = \prod_{v \sim v'} e^{\beta x_v x_{v'}}$$

Augment state space by introducing bond variables \(\{u_e\}\) taking values in \([0, e^\beta]\) and consider

$$\pi(x, u) \propto \prod_{e = (v, v') \in E} 1 \left\{ 0 \leq u_e \leq e^{\beta x_v x_{v'}} \right\}$$

- Marginal distribution is \(\pi(x)\)
- Conditional distributions
  - \(\pi(u | x)\) is a product of uniform dist. (with range depending on two neighboring spins)
  - \(\pi(x | u)\)

: if \(\begin{cases} u_e > e^{-\beta} & \Rightarrow x_v = x_{v'} \\ u_e \leq e^{-\beta} & \Rightarrow \text{no constraints} \end{cases}\) \(\therefore \pi(x | u) \propto \prod_{e : u_e > e^{-\beta}} 1(x_v = x_{v'})\)
Clustering

- Based on $u$: cluster sites according to whether they have a mutual bond: i.e. $u_e > e^{-\beta}$
- All sites in a cluster should take identical values
- Conditional on clusters, all configurations that do not violate the cluster homogeneity are equally likely
Simpler augmented model

- Only use auxiliary bonding variable \( b_e = 1 \{ u_e > e^{-\beta} \} \)

\[
\pi(x, b) \propto \prod_{e: x_v \neq x_{v'}} 1(b_e = 0) \prod_{e: x_v = x_{v'}} \left[ 1(b_e = 0) + (e^{2\beta} - 1)1(b_e = 1) \right]
\]

- Clustering done by connecting all neighboring sites with bond value 1

- Conditional on \( b \), spin value of one cluster independent of the other clusters
Swendsen-Wang algorithm [1987]

Iterate between sampling from $\pi(b \mid x)$ & $\pi(x \mid b)$

1. For given spin configuration $x$, form bond variables

$$b_e = \begin{cases} 
1 \ & \text{wp } \ 1 - e^{-2\beta} \ & \text{if } x_v = x_v' \\
0 \ & \text{if } x_v \neq x_v' 
\end{cases}$$

$$b_e = 0 \quad \text{if } x_v \neq x_v'$$

2. Conditional on $b$, update spins by sampling uniformly on all compatible configurations; i.e. clusters take on iid $\text{Ber}(1/2)$ values (every cluster flipped wp 1/2)

Clusters connect neighboring sites with bond value 1
Numerical example

Swendsen-Wang algorithm (click link)
Wolff’s algorithm

Wolff (1989) introduced a modification which significantly enhances the SW algorithm

▶ For a given configuration \( x \), randomly pick a site \( v \) & grow recursively a bonded set from it

- Check all the unchecked neighboring sites of a current set \( C^{\text{old}} \); add a bond between a neighboring site and \( C^{\text{old}} \) in the same way as in the SW algorithm

- Add newly bonded sites to \( C^{\text{old}} \) & form \( C^{\text{new}} \)

- Stop recursion when there is no unchecked site to add. Final cluster is \( C \)

▶ Flip all the signs in \( C \) (no random sampling)
Difference with SW

In each iteration

- Only one cluster is constructed
- All spins are changed
Interpretation as metropolis algorithm

Suppose $C$ has $n + m$ neighboring sites

\[ n \text{ links to } -1 \quad m \text{ links to } +1 \]

If $C$ is all $1 \implies$ flipping to $-1$

Probability ratio

\[
\frac{\mathbb{P}(\text{new})}{\mathbb{P}(\text{old})} = \frac{e^{-\beta \sum_v x_v}}{e^{+\beta \sum_v x_v}} = \frac{e^{-\beta(m-n)}}{e^{\beta(m-n)}} = e^{-2\beta(m-n)}
\]
Consider process of building $C$ (proposal)

\[
P(\text{old} \to \text{new}) \frac{P(\text{new} \to \text{old})}{P(\text{new} \to \text{old})} = P(\text{breaking } m \text{ bonds}) \frac{e^{-2\beta m}}{e^{-2\beta n}} = e^{-2\beta(m-n)}
\]

Conclusion:

\[
\frac{P(\text{new})P(\text{new} \to \text{old})}{P(\text{old})P(\text{old} \to \text{new})} = e^{-2\beta(m-n)}e^{2\beta(m-n)} = 1
\]

Metropolis always accepts the move!